Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information for:

Fluorescence response of cruciform D-π-A-π-D phenothiazine derivatives to mechanical force

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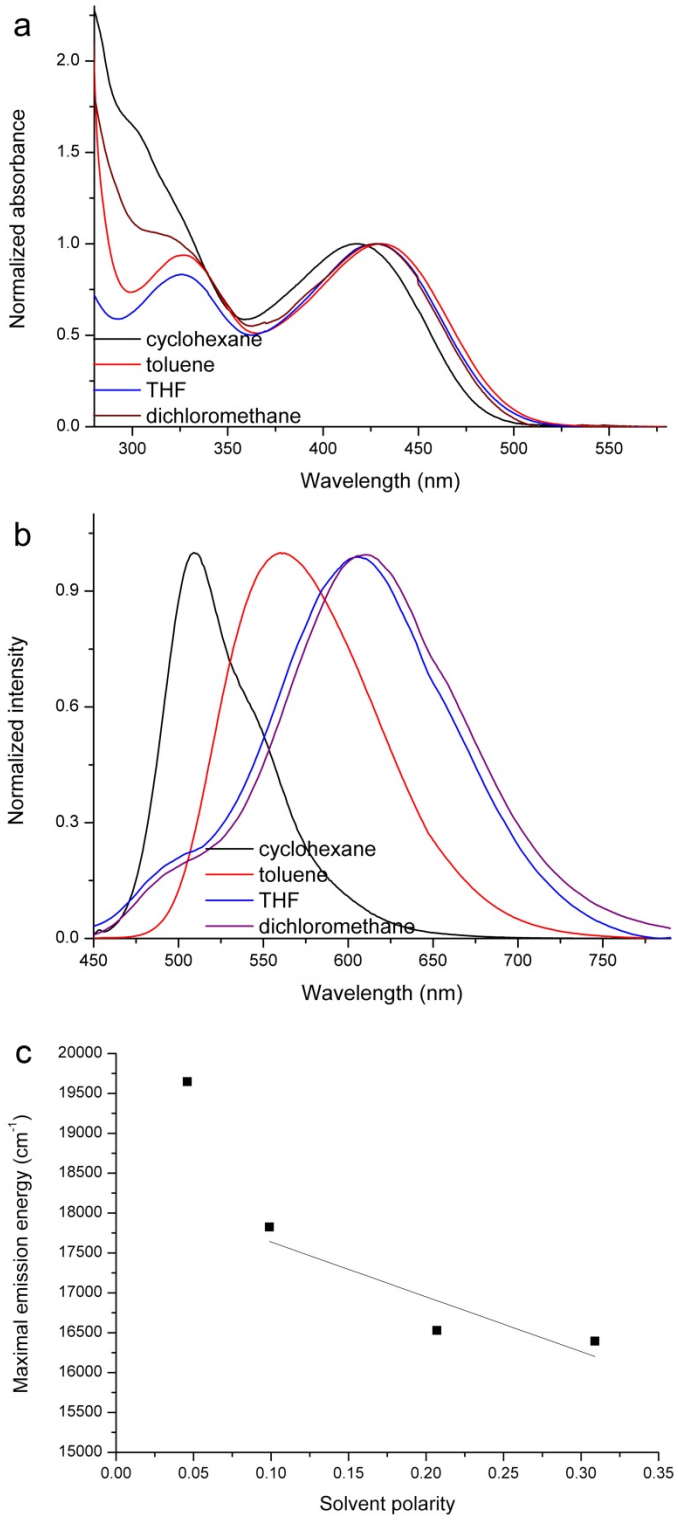

Fig. S1 (a) Absorption and (b) fluorescence spectra of EPTD in different solvents. c) Lippert–Mataga plot: fluorescence emission maximum energy of EPTD as a function of solvent polarity. λ_{ex} = 400 nm. C = 5×10^{-5} M.

Table S1. Photophysical data of EPTD in different solvents.

	Cyclohexane	Toluene	THF	CH_2Cl_2
λ_{abs} (nm)	417	430	428	428
λ_{em} (nm)	509	561	605	609

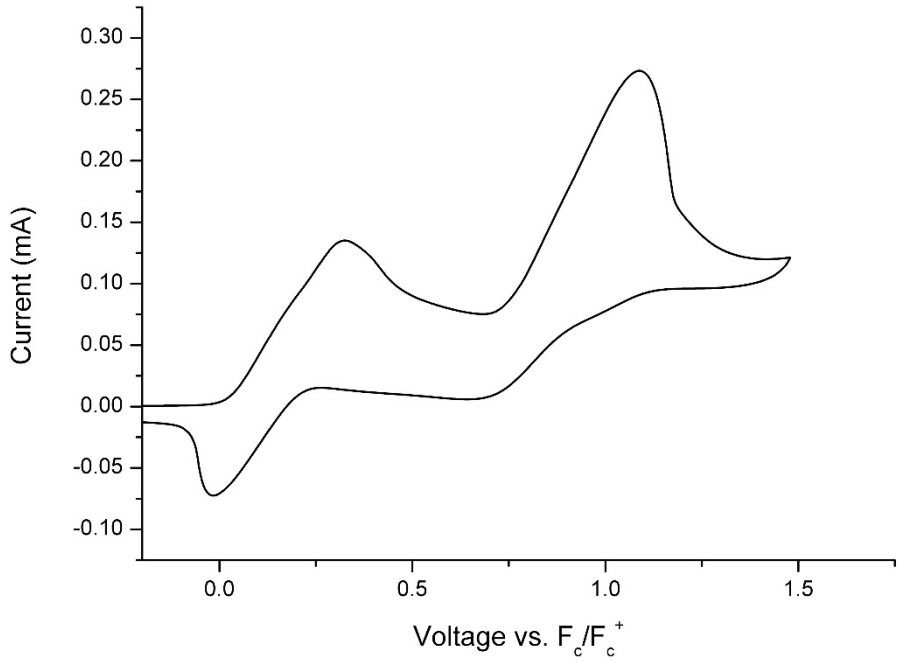

Fig. S2 Cyclic voltammetry curve of EPTD in dry THF at a scan rate of 0.1V/s.

Table S2. Photophysical data of EPTD in THF and energy levels obtained by cyclic voltammogram and quantum chemical calculation based on EPTD-E.

	λ_{abs}[a] (nm)	λ_{onset}[a] (nm)	E_g[b] (eV)	HOMO[c] (eV)	LUMO[d] (eV)	HOMO[e] (eV)	LUMO[e] (eV)
EPTD	325, 417	482	2.57	-4.95	-2.38	-4.81	-2.17

[a] Measured in THF (10^{-5} M); [b] E_g was determined from the edge of the absorption spectrum. [c] HOMO energy level was obtained by first oxidation peak in DMF with ferrocene/ferrocenium (F_c/F_c^+) as an internal reference. [d] $E_{LUMO} = E_{HOMO}+E_g$. [e] DFT calculated at theoretical level of B3LYP/6-31G.

Table S3. Photophysical data of EPTD in vacuum obtained by quantum chemical calculation.

	Transition	Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
EPTD	$S_0 \rightarrow S_1$	HOMO-2→LUMO (9.2 %) HOMO-1→LUMO+2 (3.5 %) HOMO→LUMO (82.4%)	3.0316	408.97	1.6087

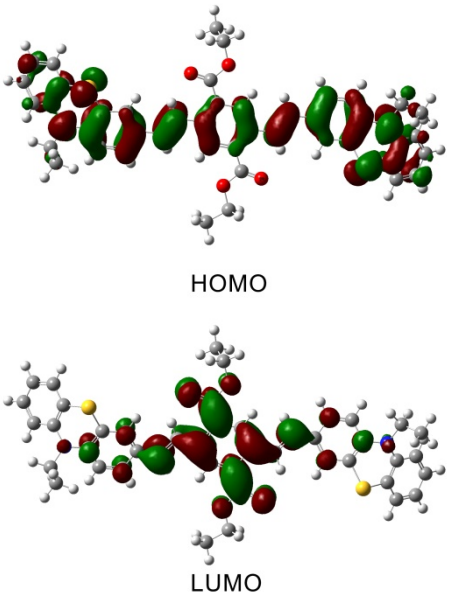

Fig. S3 Frontier orbitals of EPTD optimized in vacuum.

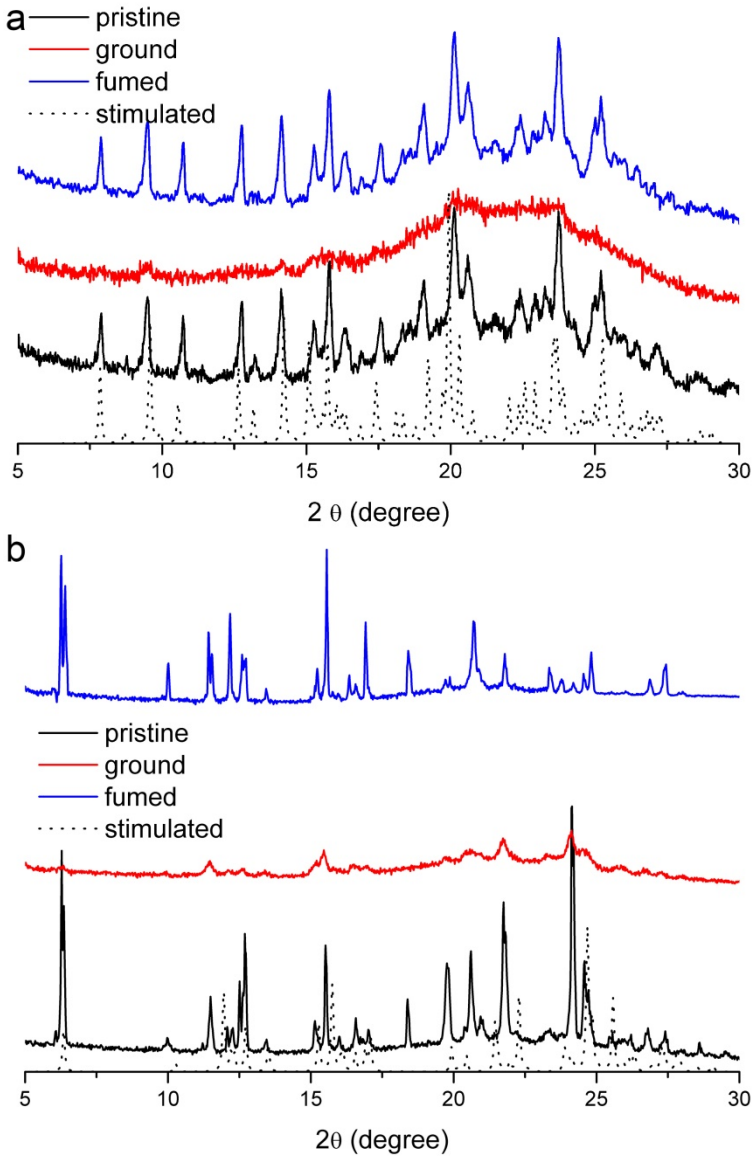

Fig. S4 XRD patterns of (a) EPTD-Y and (b) EPTD-R in pristine crystals, ground and fumed solids. Dot lines are stimulated XRD patterns.

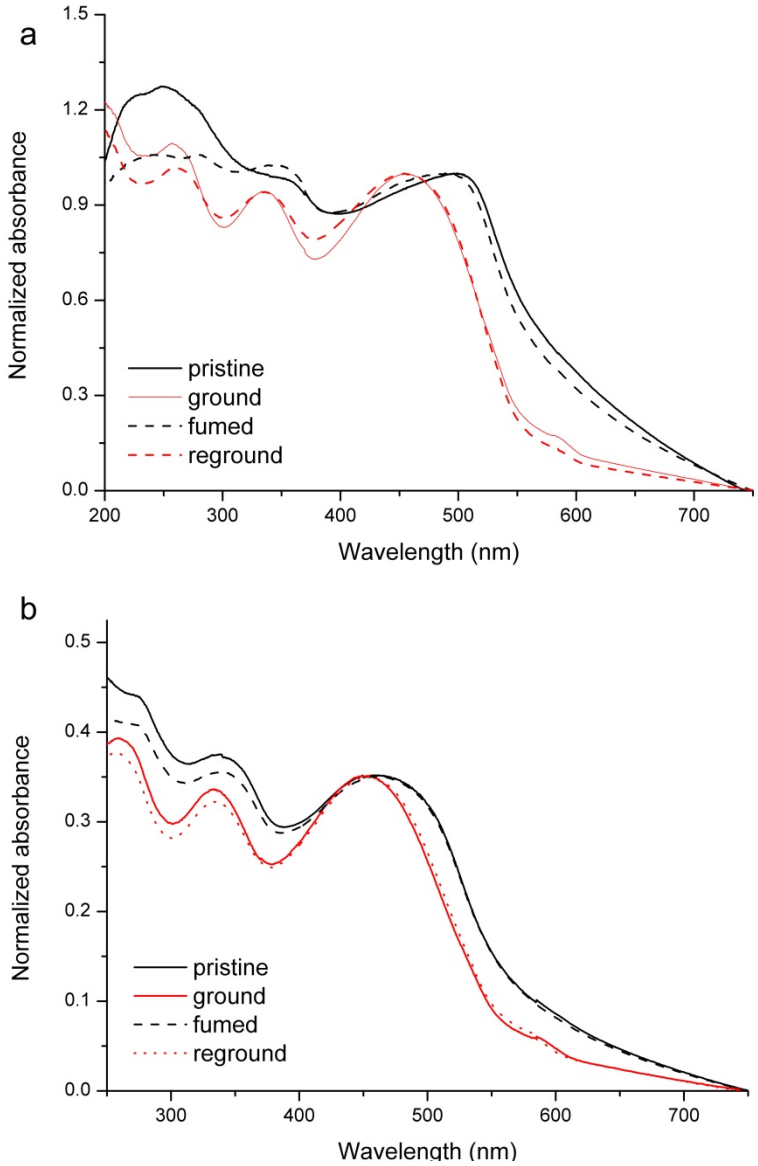

Fig. S5 UV-Vis absorption spectra of (a) EPTD-Y and (b) EPTD-R in different states.

Table S4. Photophysical data of EPTD in Z-form and E-form obtained by quantum chemical calculation.

	Dipole moment (Debye)	Transition	Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
Z-form	4.79	$S_0 \rightarrow S_1$	HOMO-2→LUMO (9.6 %) HOMO-1→LUMO+2 (7.5 %) HOMO→LUMO (73.7 %)	3.5384	350.39	1.8105
E-form	0	$S_0 \rightarrow S_1$	HOMO-2→LUMO (12.1 %) HOMO-1→LUMO+2 (5.4 %) HOMO→LUMO (75.0 %)	3.5055	353.69	1.4926

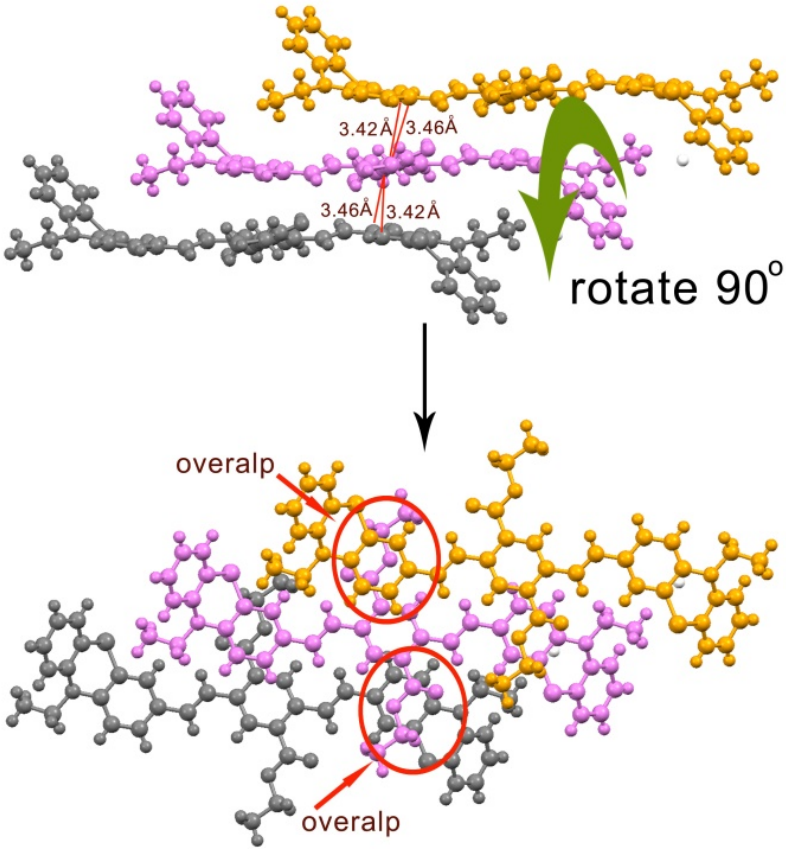

Fig. S6 Molecular stacking and the interaction between ester groups and phenothiazine moieties in EPTD-R crystal.

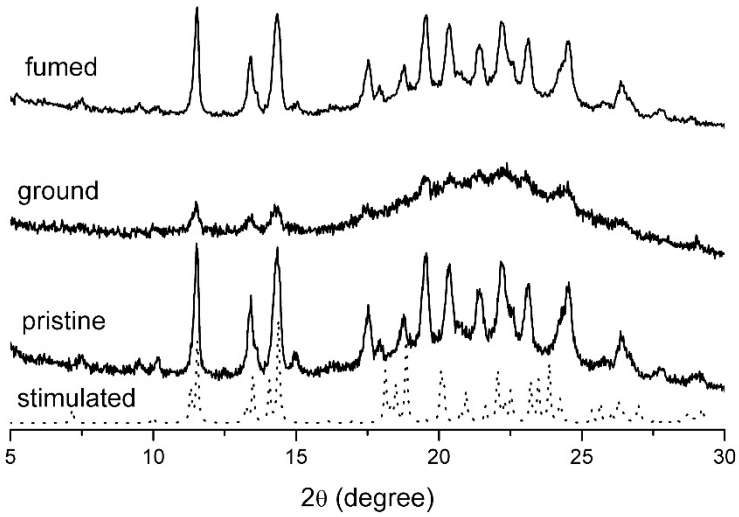

Fig. S7 XRD patterns of BPTD in different states.

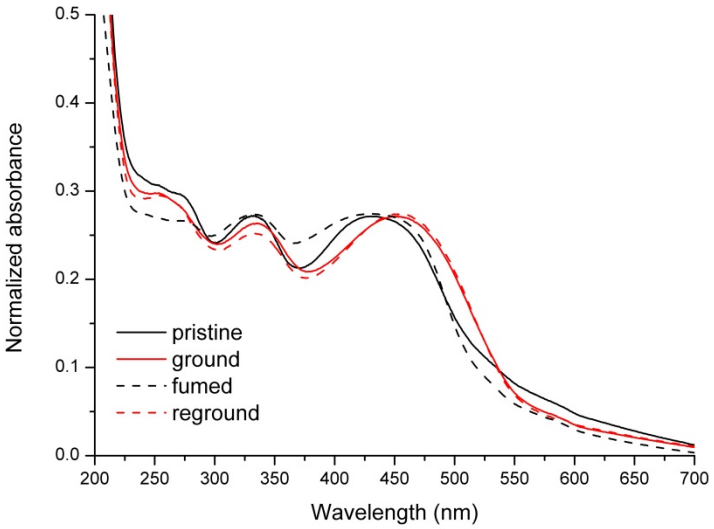

Fig. S8 UV-Vis absorption spectra of BPTD in different states.